

# Generalized Fokker-Planck equation with time dependent temperature

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ABSTRACT. A microscopic model used to derive the generalized Langevin equation for a brownian particle in a heat bath with time dependent temperature is improved to construct and solve the corresponding Fokker-Planck equation.

RESUMEN. Utilizando un modelo microscópico se obtiene la ecuación de Langevin generalizada para el caso de una partícula browniana sumergida en un baño térmico con dependencia temporal en la temperatura. Con dicha ecuación se construye y resuelve la ecuación de Fokker-Planck correspondiente.

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## 1. INTRODUCTION

Recently Brey and Casado have derived a generalized Langevin equation (GLE) to describe the time evolution of a Brownian particle which is in a heat bath with time dependent temperature [1]. The model corresponding to a constant temperature has been studied for a long time and it consists of a one dimensional chain of oscillators of mass  $m$  to simulate the bath. Those are coupled with a particle of mass  $M \gg m$  which is going to simulate the system [2-5]. It is well known that in this problem the bath coordinates and momenta are eliminated to obtain the evolution of the system. The stochasticity of such a model comes when the initial conditions for the bath particles are assumed to be distributed canonically with a constant temperature  $T$ , whereas the initial conditions for the system are fixed. Brey *et al.* in fact modified the bath equations to consider canonical equilibrium with a time dependent temperature  $T(t)$ , which is imposed by external means. The corresponding GLE contains this temperature besides the characteristic properties of the system.

We recall that in the limit of a great number of oscillators in the bath, their normal frequencies can be distributed according to different models [6,7]. In fact a Debye type of frequency distribution drives to a Langevin equation with time dependent coefficients. A Lorentzian distribution can be used to simulate the hydrodynamic modes in a fluid and this case drives to an Ornstein-Uhlenbeck noise for the system, with the corresponding GLE. In this work we shall consider the Lorentzian distribution for the bath modes together with a time dependent temperature. The GLE becomes a non-Markovian equation which will be written in an enlarged space of variables in order to derive the corresponding

Fokker-Planck equation. In the last step we shall solve it for a given set of initial conditions for the brownian particle.

## 2. GENERALIZED LANGEVIN EQUATION

To start with our treatment we will write the equations corresponding to the bath particles, which in fact are not derivable from a Hamiltonian as it is usual in this kind of treatments. Instead they are modified in order to allow the time dependence in the external temperature, those equations were proposed in the literature and have dissipative contributions coupled with the generalized coordinates and momenta of particles in the thermal bath [1]:

$$\frac{d}{dt}q_i(t) = \frac{p_i(t)}{m_i} + \alpha(t)q_i(t), \quad (1)$$

$$\frac{d}{dt}p_i(t) = -m_i\omega_i^2 \left( q_i(t) - \gamma_i \frac{Q(t)}{\omega_i^2} \right) + \alpha(t)p_i(t), \quad (2)$$

$q_i(t)$  and  $p_i(t)$  are the coordinates and momenta of the bath particles,  $m_i$  their mass,  $\omega_i$  the frequencies,  $Q(t)$  the coordinate of the Brownian particle,  $\gamma_i$  are the coupling functions between the particle and the bath and  $\alpha(t) = \frac{1}{2} \frac{d}{dt} \ln T(t)$  contains the temperature of the bath, which is a well behaved function of time.

Equations (1-2) are constructed in such a way that the bath particles are always in a canonical equilibrium associated with the time dependent temperature, allowing for continuous cooling or heating of the system. Notice should be made that the initial conditions in the bath particles imply a Gaussian distribution function for these quantities, with a temperature given by  $T(0)$ . Then the time dependent temperature  $T(t)$  is lighted on and the bath follows it in a canonical way. The resulting equations are easily solved in terms of the initial conditions for the bath, in such a way that they can be substituted in a direct way into the equations of motion for the Brownian particle:

$$\frac{dQ(t)}{dt} = \frac{P(t)}{M}, \quad (3)$$

$$\frac{dP(t)}{dt} = -U'(Q) - \int_0^t \zeta(t-t') \left( \frac{T(t)}{T(t')} \right)^{\frac{1}{2}} \left( \frac{P(t')}{M} - \alpha(t)Q(t') \right) dt' + \mathcal{F}(t). \quad (4)$$

Here  $P(t)$  is the generalized momentum of the particle,  $U(Q)$  the external potential acting on it,  $\zeta(t-t')$  depends on the coupling functions  $\gamma_i$  and the normal frequencies  $\omega_i$ ,

$$\zeta(t-t') = \sum_{i=1}^{i=N} m_i \frac{\gamma_i^2}{\omega_i^2} \cos[\omega_i(t-t')]. \quad (5)$$

Lastly  $\mathcal{F}(t)$  can be written in terms of the initial conditions, namely

$$\mathcal{F}(t) = \left(\frac{T(t)}{T(0)}\right)^{\frac{1}{2}} \left[ \sum_1^N \gamma_i m_i \left( q_i(0) - \gamma_i \frac{Q(0)}{\omega_i^2} \right) \cos \omega_i t + \gamma_i \frac{p_i(0)}{\omega_i} \sin \omega_i t \right]. \quad (6)$$

Equations (3–6) give us the generalized Langevin description for the Brownian particle, where  $\zeta(t - t')$  plays the role of the dissipation and  $\mathcal{F}(t)$  is the fluctuating force, whose statistical properties corresponds to a Gaussian noise and its nontrivial averages are given by

$$\langle \mathcal{F}(t) \rangle = 0, \quad (7)$$

$$\langle \mathcal{F}(t)\mathcal{F}(t') \rangle = K_B [T(t)T(t')]^{\frac{1}{2}} \zeta(t - t'). \quad (8)$$

When we assume the number of oscillators  $N$  is very large, we can go to the continuous limit and introduce a distribution of frequencies. In fact if this distribution is assumed to be a Lorentzian one, we have a simulation of hydrodynamic modes in a fluid [6],

$$g(\omega) = \frac{2N}{\pi\tau} \frac{1}{(\omega^2 + \tau^{-2})}. \quad (9)$$

Here we have taken all masses of oscillators equal to  $m$  and  $\tau$  represents the relaxation time of the corresponding hydrodynamic mode, giving us a cutoff frequency. In this case the coupling functions must depend on the frequency and the number of oscillators  $N$ , in order to have a finite correlation in the limit  $N \rightarrow \infty$  namely,

$$\gamma(\omega) = \gamma_0 \frac{\omega}{\sqrt{N\tau}}. \quad (10)$$

With these assumptions the correlation of the fluctuating force becomes an exponential function characteristic of a Gaussian Ornstein-Uhlenbeck noise:

$$\zeta(t - t') = m \frac{\gamma_0^2}{\tau} \exp\left(-\frac{|t - t'|}{\tau}\right). \quad (11)$$

The GLE corresponding to the Brownian particle is then written as follows:

$$\frac{dP(t)}{dt} = -U'(Q) - \int_0^t \zeta(t - t') \left( \frac{d}{dt'} \frac{\mathcal{R}(t')}{\mathcal{R}(t)} Q(t') \right) dt' + \mathcal{F}(t), \quad (12)$$

where  $\mathcal{R}(t) = \left(\frac{T(0)}{T(t)}\right)^{\frac{1}{2}}$ .

It is obvious that this problem is a non-Markovian one [8] and the construction of a Fokker-Planck equation must be done in an indirect way.

3. GENERALIZED FOKKER-PLANCK EQUATION

First of all let us define a new space of variables to study the behavior of the Brownian particle, this space will be composed of the coordinate, momentum and an extra variable with the meaning of a force  $(Q, P, S)$ . The new variable is chosen in such a way that the new set of Langevin type equations will contain a Gaussian delta correlated noise, namely

$$\begin{aligned} \frac{dQ(t)}{dt} &= \frac{P(t)}{M}, \\ \frac{dP(t)}{dt} &= -U'(Q) + S(t), \end{aligned} \tag{13}$$

$$\frac{dS(t)}{dt} = \frac{m\gamma_0^2}{\tau} \alpha(t)Q(t) - \frac{\gamma_0^2}{\tau} \frac{mP(t)}{M} + \left(\alpha(t) - \frac{1}{\tau}\right) S(t) + \Gamma(t), \tag{14}$$

where  $\Gamma(t)$  is the new noise and its statistical properties are the following ones:

$$\langle \Gamma(t) \rangle = 0, \quad \langle \Gamma(t)\Gamma(t') \rangle = \frac{2mK_B T(t)\gamma_0^2}{\tau^2} \delta(t - t'). \tag{15}$$

Equation (15) shows how the intensity of the noise contains the time dependent temperature, among other parameters of our problem.

This set of equations is now ready to be the starting point in the derivation of the Fokker-Planck equation, since the drift and diffusion coefficients are immediately identified:

$$\begin{aligned} \frac{\partial}{\partial t} W(Q, P, S; t) &= -\frac{P}{M} \frac{\partial}{\partial Q} W(Q, P, S; t) + [U'(Q) - S] \frac{\partial}{\partial P} W(Q, P, S; t) \\ &+ \frac{\partial}{\partial S} \left[ \left[ \frac{m\gamma_0^2}{\tau} \left( -\alpha(t)Q + \frac{P}{M} \right) + \left( -\alpha(t) + \frac{1}{\tau} \right) S \right] W(Q, P, S; t) \right] \\ &+ \frac{mK_B T(t)\gamma_0^2}{\tau^2} \frac{\partial^2}{\partial S^2} W(Q, P, S; t). \end{aligned} \tag{16}$$

Notice should be made that the external force is an arbitrary one and the Fokker-Planck equation is influenced by the characteristics of the heat bath through  $m$  and  $\tau$ , the coupling of the bath with the Brownian particle through  $\gamma_0$  and the time dependent temperature  $T(t)$ . This special characteristic has driven us to an equation with time dependent coefficients. However if we recall that our original noise is a Gaussian one, we hope a Gaussian solution for  $W(Q, P, S; t)$  because all couplings and transformations we have made are linear ones [9]. Then for a set of specified initial conditions for the Brownian particle we can write the following solution:

$$W(Q, P, S; t) \sim \exp \left[ -\frac{1}{2} \sum_{i,j} \mathbf{M}_{ij}(t)(x_i - a_i(t))(x_j - a_j(t)) \right], \quad i, j = Q, P, S; \tag{17}$$

where  $M_{ij}$  is a symmetric positive definite matrix representing the fluctuations of the variable and  $a_i(t)$  are their corresponding averages. The values of these quantities satisfy the following equations:

$$\frac{d}{dt}a_i(t) - \sum_j \mathbf{A}_{ij}(t)a_j(t) = 0, \tag{18}$$

$$\frac{d}{dt}M_{kl}(t) + \sum_i 2\mathbf{A}_{ik}(t)M_{il}(t) + \sum_{i,j} \mathbf{B}_{ij}(t)M_{il}(t)M_{jk}(t) = 0, \tag{19}$$

where matrices  $\mathbf{A}$  and  $\mathbf{B}$  can be identified from Eq. (16) when it is written in its canonical form,

$$\frac{\partial}{\partial t}W(x_1, x_2, \dots, x_n, t) = - \sum_{i,j} \mathbf{A}_{ij} \frac{\partial}{\partial x_i}(x_j W) + \frac{1}{2} \sum_{i,j} \mathbf{B}_{ij} \frac{\partial^2 W}{\partial x_i \partial x_j}; \tag{20}$$

then the nonzero elements of matrices  $\mathbf{A}$  and  $\mathbf{B}$  are given as follows:

$$A_{QP} = \frac{1}{M}, \quad A_{PS} = 1, \tag{21}$$

$$A_{QS} = m\gamma_0^2 \frac{\alpha}{\tau}, \quad A_{PS} = -\gamma_0^2 \frac{m}{M\tau}, \quad A_{SS} = \alpha - \frac{1}{\tau},$$

$$B_{SS} = 2K_B \frac{T(t)}{\tau^2} m\gamma_0^2. \tag{22}$$

Substitution of Eqs. (21-22) in Eq. (19) allows a solution for matrix  $\mathbf{M}$ , which can be written as follows:

$$M_{kl}(t) = C_{kl}(t) \frac{d}{dt} \ln g(t), \tag{23}$$

where

$$g(t) = b_0 \int_0^t \exp \left[ - \int_0^{t'} \frac{4K_B T(t'')\gamma_0^2 m}{\tau^2} C_{SP}(t'') dt'' + \frac{2t'}{\tau} \right] dt', \tag{24}$$

and all  $C_{kl}(t)$  functions can be written in terms of  $C_{SP}(t)$  which satisfies a cubic equation given by

$$y^3 + 2 \left( \alpha - \frac{1}{\tau} \right) y^2 + \left[ \left( \alpha - \frac{1}{\tau} \right)^2 + \frac{\gamma_0^2 m}{\tau M} \right] y - \frac{\gamma_0^2 m}{M\tau^2} = 0, \tag{25}$$

where the variable  $y$  is given by

$$y = \frac{2K_B T(t)m\gamma_0^2}{\tau^2} C_{SP}(t); \tag{26}$$

all other quantities are given in the Appendix.

Just as an example of how the elements of matrix  $\mathbf{M}$  look like, we give here the explicit value of  $\mathbf{M}_{SS}(t)$  which represents the width corresponding to the new variable  $S$ :

$$\mathbf{M}_{SS}(t) = \frac{\tau^2}{2m\gamma_0^2 K_B T(t)} \frac{\exp \left[ -\frac{4K_B\gamma_0^2}{\tau^2} \int_0^t T(t') \mathbf{C}_{SP}(t') dt' \right]}{\int_0^t \left( \exp \left[ -\frac{4K_B\gamma_0^2}{\tau^2} \int_0^{t'} T(t'') \mathbf{C}_{SP}(t'') dt'' \right] \right) \exp \left( -\frac{2|t-t'|}{\tau} \right) dt'}, \quad (27)$$

where it is seen explicitly the role played by the time dependent temperature.

#### 4. CONCLUDING REMARKS

The model proposed in this work as well as its solution in terms of a Gaussian distribution function, can be studied for several limiting cases. First of all we can find the Markovian limit when the relaxation time associated with the noise is taken to be zero, then Brey and Casado's equation is obtained. The solution of the Fokker-Planck equation for this particular case can also be obtained by the method used in this paper. On the other hand, the case where the mass ratio  $\frac{m}{M} \ll 1$  simplifies the solution to a certain extent by means of a perturbative solution of Eq. (25) (see Ref. [10]). The solution as it stands describes a non-Markovian problem in terms of an extended space of variables which carries the influence of the external time dependent temperature. Its application to a particular problem will depend on the specific function of time chosen to heat or cool the system by external means.

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#### APPENDIX

The matrix  $\mathbf{C}_{ij}(t)$  is symmetric and all its elements can be written in terms of  $\mathbf{C}_{SP}(t)$ , which is the quantity we have chosen to work with. They are given by

$$\mathbf{C}_{QQ}(t) = \frac{\gamma_0[\alpha(t)]^2}{2K_B T(t)m} \left[ y + \left( \alpha - \frac{1}{\tau} \right) \right]^{-2}, \quad \mathbf{C}_{QP}(t) = \frac{\alpha(t)\gamma_0^2 \mathbf{C}_{SP}(t)}{\tau} \left[ y + \left( \alpha - \frac{1}{\tau} \right) \right]^{-1},$$

$$\mathbf{C}_{QS}(t) = \frac{\alpha(t)\tau}{2K_B T(t)m} \left[ y + \left( \alpha - \frac{1}{\tau} \right) \right]^{-1}, \quad \mathbf{C}_{PP}(t) = y \mathbf{C}_{SP}(t),$$

$$\mathbf{C}_{SS}(t) = \frac{\tau^2}{2K_B T(t)m\gamma_0^2}.$$

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